3-Methyl-1-nitrobutane

627-67-8 | DTXSID90211769

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 7.80

Global applicability domain: Inside

Local applicability domain index: 5.66e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

Image not found
Thiophene
Measured: 8.91
Predicted: 6.68

Image not found
2-Nitropropane
Measured: 8.32
Predicted: 7.41

Image not found
1,2-Dibromoethane
Measured: 15.1
Predicted: 13.4

Image not found
Thiophene, 3-methyl-
Measured: 5.25
Predicted: 7.49

Image not found
Nitrobenzene
Measured: 4.68
Predicted: 8.00